Subject: Re: ChemAxon calculated properties
Posted by MussaQ on Fri, 05 Dec 2014 19:15:34 GMT
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Thank you very much for your detailed reply, but I am still cannot access the pKa option.

I tried 2 options, in both cases the files were placed in the same directory as datawarrior.jar

1) Easy method; I searched all .jar files in the chemaxon folder under the applications folder on a Mac OSX, extracted them all and then re-zipped them and called it capka.jar (167MB file!)

2)Option 3, pasted all the .jar files i found and added their names to the Info.plist accordingly, datawarrior took longer than usual to load but no luck.

I am not familiar (brave) enough with scripting to attempt the second (difficult) option. However, would it be possible if you could provide the list of files that did work for you? so that I can cross reference with the files I found.